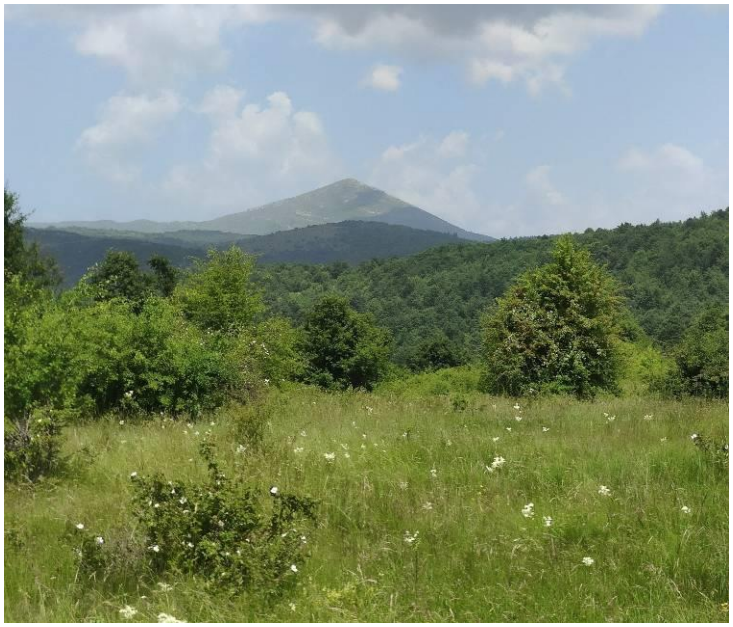
Serbian Society of Soil Science

University of Belgrade, Faculty of Agriculture

BOOK OF ABSTRACTS

3rd International and 15th National Congress

SOILS FOR FUTURE UNDER GLOBAL CHALLENGES



21–24 September 2021

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CHEMOMETRICS FOR SOIL POLLUTION MONITORING

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Abstract

Chemometrics, defined as mathematics and statistics in chemistry, has been widely present in soil pollution monitoring studies for quite some time. The chemometric approach incorporates a large number of algorithms and models. In most cases, chemometric methods are used to optimize the measurement procedures to gather soil pollution monitoring data or to elucidate qualitative and quantitative relationships within these data, which may be quite complex and be overlooked when using classical methodologies. Soil pollution monitoring involves the processes of sampling and analyzing specific toxic pollutants, such as heavy metal(loid)s, polycyclic aromatic hydrocarbons (PAH), polychlorinated biphenyls (PCB), petroleum hydrocarbons, pesticides, and radionuclides. With the help of modern analytical techniques, the spatial and temporal changes in concentrations of these pollutants usually generate a vast amount of data. In order to achieve meaningful soil monitoring, both sampling/analysis and data assessment procedures must be carefully planned and performed. This often includes factorial design strategies for experiment optimization. Two factorial designs, one used for screening the selected parameters and the other used for their optimization, are usually used together. Alternatively, a sequential optimization may be made by applying the Simplex algorithm. On the other hand, among the most used chemometric methods for soil pollution monitoring data evaluation, two groups can be distinguished: supervised and unsupervised pattern recognition methods. In supervised methods, input and output data are known, and the primary goal is to find the relationship between inputs and outputs. These methods are most often used in classification so that the soil sample joins an already defined group. There is also an application in regression, where the input values of soil contaminant predict the output result. This group includes partial least squares regression (PLS), discriminant analysis (DA), artificial neural network (ANN), support vector machines (SVM). In unsupervised methods, no prior knowledge of any relationship in the soil pollution dataset is required. The aim is to identify the underlying structure within the dataset. These methods are commonly used for dimensionality reduction and exploratory analysis. The following unsupervised methods are frequently used: principal component analysis (PCA), cluster analysis (CA), positive matrix factorization (PMF), and Kohonen self-organizing maps (SOM). In addition to the chemometric tools mentioned above, geographic information system (GIS) analysis protocols, such as spatial autocorrelation, inverse distance weighted interpolation, and kriging, are unavoidable in soil pollution monitoring.

Keywords: multivariate, classification, GIS, trace, PCA, source.

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